Determination of the Lower Bounds of the Goal Function for a Single-Machine Scheduling Problem on D-Wave Quantum Annealer

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Abstract. The fundamental problem of using metaheuristics and almost all other approximation methods for difficult discrete optimization problems is the lack of knowledge regarding the quality of the obtained solution. In this paper, we propose a methodology for efficiently estimating the quality of such approaches by rapidly – and practically in constant time – generating good lower bounds on the optimal value of the objective function using a quantum machine, which can be an excellent benchmark for comparing approximate algorithms. Another natural application is to use the proposed approach in the construction of exact algorithms based on the Branch and Bound method to obtain real optimal solutions.

Keywords: Quantum Annealing · Lower Bound · Scheduling

1 Introduction

The concept of quantum computing and computers was independently introduced in the early 1980s. Since then, it has soaked up very significant developments in theory and, most importantly, in the last 20 years, in machines implementing quantum computing paradigms. Currently, the two leading types of quantum machines are quantum gate-based computers, developed mainly by IBM and Google, and adiabatic quantum computing (AQC), developed by D-Wave and NEC. In the gate-based model, calculations are performed by applying unitarity gates to quantum bits (i.e. qubits), whose states can be read out at the end of the calculation. In contrast, in AQC, in particular quantum annealing, a

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starting state of the system modeled in hardware on multiple qubits is prepared as the ground state of the Hamiltonian encoding the solution to the desired optimization problem, to which adiabatic evolution is then applied, aiming at the minimal-energy state of the whole system. Most importantly, it is shown that the AQC is polynomially equivalent to a universal gate-based quantum computer, since any quantum circuit can be represented as a time-dependent Hamiltonian with at most polynomial charge [1].

There are quite a few descriptions in the literature of transforming classical NP-hard combinatorial optimization problems into forms suitable for quantum annealers [3]. These can be represented in Ising form using a $-1, 1$ basis (representing spins), or as a quadratic unconstrained binary optimization (QUBO) problem using a binary basis. These two forms are equivalent. This makes it easy to solve difficult discrete optimization problems – with some (unknown) – approximation. However, there is so far no description in the literature of methods that can quickly indicate the error of such an approximation. In this paper, we try to fill this research gap by proposing the idea of determining a lower bound on the value of the objective function of an optimization problem by solving with quantum annealing a dual problem resulting from Lagrange relaxation.

2 Formulation of the Problem

We will present the method of constructing a lower bound on the D-Wave quantum machine using the example of the NP-hard single-machine Total Weighted Tardiness Problem (TWTP), denoted in the literature by $1||\sum w_i T_i$. There is given a *set of tasks* $\mathcal{J} = \{1, 2, ..., n\}$, which must without interruption be executed on a single-machine. The start of the tasks begins at time 0. At any time, a machine can execute at most one task. The following are associated with each task $i \in \mathcal{J}$: *execution time* p_i, *critical line* d_i, and *weight of penalty function* w_i. For a fixed order of execution of tasks on the machine, let S_i be the starting moment and $C_i = S_i + p_i$ the ending moment of the execution of task $i \in \mathcal{J}$. Then, *delay* $T_i = \max\{0, C_i - d_i\}$, and *cost of tardiness* (*penalty*) $f_i(C_i) = w_i \cdot T_i$. The TWTP problem considered in this paper consists in determining the execution schedule of the machine described by S_i, C_i, $i \in \mathcal{J}$ with a minimal *total cost* $\sum_{i=1}^{n} f_i(C_i) = \sum_{i=1}^{n} w_i T_i$.

The task execution schedule described by the sequences S_i, C_i, $i \in \mathcal{J}$ is feasible if the following constraints are met:

$$S_i + p_i \leq S_j \vee S_j + p_j \leq S_i, \; i \neq j, \; i, j = 1, 2, \ldots, n, \tag{1}$$

$$S_i \geq 0, \;\; C_i = S_i + p_i, \;\; i = 1, 2, \ldots, n. \tag{2}$$

The single-machine problem of minimizing the sum of delay costs formulated above is NP-hard. Optimal algorithms for solving the problem based on the methods of dynamic programming, i.e. on Lagrange relaxation and branch and bound, are described in the works by (Potts [6], and Wodecki [12]). These algorithms are time consuming, thus in practice, small-scale examples can be solved on classical computers with their help. These are mainly metaheuristics that have been widely used since the 1990s: tabu search (Bożejko et al. [4], Uchroński [10]), dynamic programming (Rostami et al. [9]), simulated annealing (Potts and Van Wassenhove [7]). Extensive reviews of the literature on scheduling problems with due dates was also presented by Adamu and Adewumi [2]. The literature also deals with single-machine scheduling problems with uncertain execution times or desired completion dates: Rajba and Wodecki [8], Bożejko et al. [5].

3 Determining the Lower Bound on the D-Wave Quantum Machine

The calculation of the lower bound of the objective function will be performed in two steps. In step one, for a quantum computer, using Lagrange relaxation we will define a dual optimization problem that will be maximized on a QPU. In step two, using a classical CPU, the exact value of the lower bound will be determined based on the results obtained in step one.

Let us consider a certain optimization problem having the following property: its solution (in the sense of value) is always less than or equal to the optimal one. A relaxed version of the problem considered in this paper using the Lagrange function has this property. The relaxation will be governed by the non-overlapping constraint (i.e. their decouplability), the inequality of the (1).

For simplicity of notation, let us assume that the tasks are executed in the natural order of π, $\pi(i) = i$. The TWTP problem under consideration can be written in the form of an optimization task:

$$\min_{S} \sum_{i=1}^{n} w_i T_i \tag{3}$$

subject to

$$S_i + p_i - S_j \leq K(1 - y_{ij}),\ j = i+1, \ldots, n,\ i = 1, \ldots, n, \tag{4}$$

$$S_j + p_j - S_i \leq K y_{ij},\ j = i+1, \ldots, n,\ i = 1, \ldots, n, \tag{5}$$

$$y_{ij} \in \{0, 1\},\ j = i+1, \ldots, n,\ i = 1, \ldots, n, \tag{6}$$

$$S_i \geq 0,\ i = 1, \ldots, n, \tag{7}$$

where K is some sufficiently large number. In turn, y_{ij} is a binary variable equal to 1 if the task i precedes j and 0 otherwise. The Lagrange function with multipliers u_{ij} and v_{ij}, $i, j = 1, 2, \ldots, n$ takes for the vector $S = (S_1, S_2, \ldots, S_n)$ and the matrix $y = [y_{ij}]_{n \times n}$ the form:

$$L(S, y, u, v) = \sum_{i=1}^{n} w_i T_i + \sum_{i=1}^{n} \sum_{j=i+1}^{n} u_{ij}(S_i + p_i - S_j - K(1 - y_{ij}))$$

$$+ \sum_{i=1}^{n} \sum_{j=i+1}^{n} v_{ij}(S_j + p_j - S_i - K y_{ij})$$

Transforming this expression we obtain

$$L(S,y,u,v) = \sum_{i=1}^{n} L_i(S_i,u,v) + K\sum_{i=1}^{n}\sum_{j=i+1}^{n} Q_{ij}(y_{ij},u,v) + V(u,v). \tag{8}$$

where

$$L_i(S_i,u,v) = w_iT_i + \alpha_i S_i, \quad \alpha_i = \sum_{j=i+1}^{n}(u_{ij}-v_{ij}) + \sum_{j=1}^{i-1}(v_{ji}-u_{ji}),$$

$$Q_{ij}(y_{ij},u,v) = (u_{ij}-v_{ij})y_{ij}, \quad V(u,v) = \sum_{i=1}^{n} p_i\left(\sum_{j=1}^{i-1} v_{ji} + \sum_{j=i+1}^{n} u_{ij}\right).$$

Let us note that if S^* is an optimal solution to the TWTP problem, then for *any non-negative* $u, v \geq 0$ there is a

$$\sum_{j=1}^{n} w_jT_j \geq \sum_{j=1}^{n} w_jT_j + \sum_{i=1}^{n}\sum_{j=i+1}^{n} u_{ij}(S_i^* + p_i - S_j^* - K(1-y_{ij}))$$

$$+\sum_{i=1}^{n}\sum_{j=i+1}^{n} v_{ij}(S_i^* + p_i - S_j^* - Ky_{ij}) \geq \min_{S}\min_{y} L(S,y,u,v).$$

Therefore, when looking for a good lower bound, one should compute

$$LB = \max_{u,v}\min_{S,y} L(S,y,u,v) = \max_{u,v}\left(\sum_{i=1}^{n}\min_{0\leq S_i\leq T-p_i} L_i(S_i,u,v)\right.$$

$$\left. + K\sum_{i=1}^{n}\sum_{j=i+1}^{n}\min_{y} Q_{ij}(y_{ij},u,v) + V(u,v)\right) \tag{9}$$

whereby the maximization with respect to u and v can be approximate, while that with respect to S and y is exact.

Determination of Lower Bound (Step 1) on a D-Wave Quantum Annealer. Let us note that the lower bound (9) can be written as a minimization of the opposite (minus) value, with constraints:

$$LB = -\min_{u,v,S,y}\left[-\left(\sum_{i=1}^{n} L_i(S_i,u,v) + K\sum_{i=1}^{n}\sum_{j=i+1}^{n} Q_{ij}(y_{ij},u,v) + V(u,v)\right)\right] \tag{10}$$

s.t.

$$L_i(S_i,u,v) \leq L_i(0,u,v), \; i = 1,2,\ldots,n, \tag{11}$$

$$L_i(S_i, u, v) \leq L_i(1, u, v),\ i = 1, 2, \ldots, n, \tag{12}$$

$$\vdots$$

$$L_i(S_i, u, v) \leq L_i(T - p_i, u, v),\ i = 1, 2, \ldots, n, \tag{13}$$

and

$$Q_{ij}(y_{ij}, u, v) \leq Q_{ij}(0, u, v),\ i, j = 1, 2, \ldots, n, \tag{14}$$

$$Q_{ij}(y_{ij}, u, v) \leq Q_{ij}(1, u, v),\ i, j = 1, 2, \ldots, n, \tag{15}$$

where each of the constraints (11)–(13) of the form $L_i(S_i, u, v) \leq L_i(t, u, v)$, $i = 1, 2, \ldots, n$, $n = 0, 1, \ldots, T - p_i$, where $L_i(S_i, u, v) = w_i T_i + \alpha_i S_i$ is technically written in the D-Wave machine program as one of two constraints – each of (11)–(13) is encoded as expressed in the Algorithm 1, since in the constraints of the QUBO model, there cannot be a function *maximum* resulting from the formula to calculate the delay for a task i starting at time t equalling $T_i(t) = \max\{0, t + p_i - d_i\}$.

Algorithm 1: Adding S minimalization constraints to the QUBO model

for $i = 1, 2, \ldots, n$ **do**
    for $t = 0, 1, 2, \ldots, T - p_i$ **do**
        if $(t + p_i - d_i > 0)$ **then**
            Add constraint $L_i(S_i, u, v) \leq w_i \cdot (t + p_i - d_i) + \alpha_j \cdot t$
        else
            Add constraint $L_i(S_i, u, v) \leq w_i \cdot 0 + \alpha_i \cdot t$

The task formulated in this way can already be directly implemented on a D-Wave machine since all constraints, as well as the objective function, are linear. The difficulty is the possible suboptimality of the resulting quantum annealing vector S and binary matrix y with respect to the formulation (9).

4 Experimental Research

To verify the effectiveness of the proposed method of determining the lower bound, computational experiments were carried out on the quantum algorithm implemented on the D-WAVE quantum annealer and the algorithm determining the lower bound on a classical silicon computer with an i7-12700H 2.30 GHz processor. The research was carried out on 30 instances divided into three groups of 10 instances each. Instance groups differ in the number of tasks. A full set of test instances can be found in [11].

Table 1 presents the results of experimental research, in particular, in column 1 there is LB^Q determined by the quantum algorithm, while in column 3 there is LB^{CPU} determined by the classical algorithm. Columns 2 and 4 show the time of quantum computations and computations on a classical computer, respectively. In addition, column 5 includes the acceleration of calculations and the relative difference of the LB value as a measure of the quality assessment of the generated solutions (column 6), determined as $Quality = \frac{LB^Q - LB^{CPU}}{LB^{CPU}}$. Analyzing the results presented in the Table, we can conclude that in a significant number of instances, the LB determined by the quantum annealer is significantly greater than the LB determined on a classical computer. The LB value determined by the annealer is not lower for all instances, with the LB value determined on the CPU, and in 26 out of 30 instances it is better. For the instance $wt7\_70$ LB^Q is nearly 200 times better than LB^{CPU}. The Quantity value occurs on average 17 times for the $n = 5$ group, 8 times for the group $n = 6$ and 92 times for the group $n = 7$. Comparing the calculation time of a quantum exponent and a classical computer, we can conclude that the time of quantum calculations is from 6 to nearly 140 times shorter than the time of calculations on a classical computer. The advantage of quantum computing increases as the number of tasks increases. For the $n = 5$ group, it is on average 9 times lower, while for the $n = 8$ group, it is 97 times lower on average (Fig. 1).

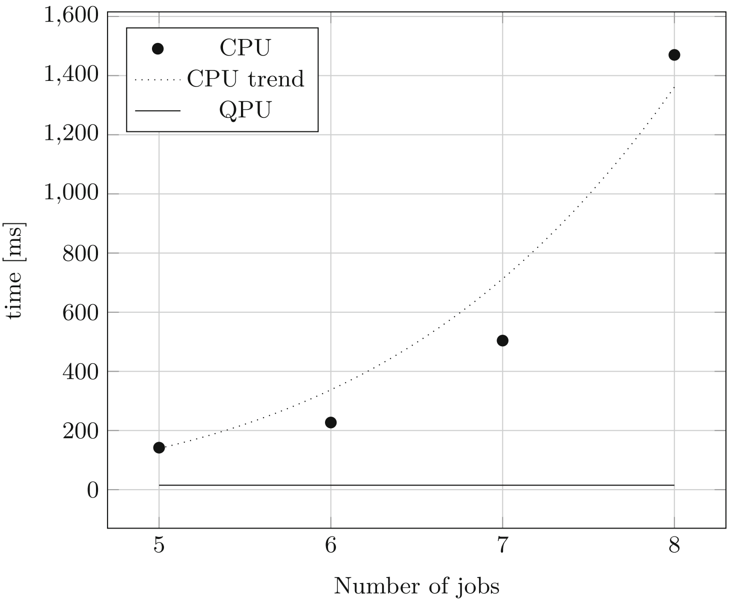

Fig. 1. Computation time of LB calculations on quantum processor QPU and silicon processor CPU

Table 1. The results of experiments.

example	LB^Q	$Time^Q$	LB^{CPU}	$TIME^{CPU}$	SPEED-UP	Quality
wt5_40	423	15	0	183	12,20	
wt5_41	2153	15	456	140	9,33	4,72
wt5_42	1657	15	300	103	6,87	5,52
wt5_43	1001	15	10	148	9,87	100,1
wt5_44	1588	15	116	115	7,67	13,69
wt5_45	2099	15	0	187	12,47	
wt5_46	1791	15	604	116	7,73	2,97
wt5_47	2443	15	783	147	9,80	3,12
wt5_48	3353	15	1138	123	8,20	2,95
wt5_49	1578	15	358	100	6,67	4,41
wt6_70	469	15	0	202	13,47	
wt6_71	3328	15	385	241	16,07	8,64
wt6_72	3563	15	290	359	23,93	12,29
wt6_73	2630	15	421	178	11,87	6,25
wt6_74	3216	15	612	312	20,80	5,25
wt6_75	1280	15	0	324	21,60	—
wt6_76	0	15	0	261	17,40	—
wt6_77	8	15	0	242	16,13	—
wt6_78	0	15	0	299	19,93	—
wt6_79	16	15	0	186	12,40	—
wt7_70	3049	15	15	450	30,00	203,27
wt7_71	3635	15	317	582	38,80	11,47
wt7_72	1395	15	0	282	18,80	—
wt7_73	3806	15	62	451	30,07	61,39
wt7_74	3117	15	0	420	28,00	—
wt7_75	2840	15	0	238	15,87	—
wt7_76	0	15	0	605	40,33	—
wt7_77	64	15	0	436	29,07	—
wt7_78	0	15	0	302	20,13	—
wt7_79	12	15	0	381	25,40	—
wt8_80	100	15	0	1407	93,80	—
wt8_81	1271	15	0	1278	85,20	—
wt8_82	992	15	0	1249	83,27	—
wt8_83	662	15	0	1576	105,07	—
wt8_84	292	15	0	945	63,00	—
wt8_85	481	15	0	1682	112,13	—
wt8_86	3522	15	0	2053	136,87	—
wt8_87	1961	15	0	1127	75,13	—
wt8_88	5529	15	0	1774	118,27	—
wt8_89	2333	15	0	1512	100,80	—

5 Summary

This paper presents an algorithm for determining the lower bound on the value of the objective function for the TWTP problem implemented on a D-Wave quantum computer. The presented approach can be adapted to estimate the value of the optimal solution of other NP-hard discrete optimization problems, such as the commutator problem or multi-machine problems (e.g. job shop). A natural direction for further research will be to apply the proposed method for determining lower bounds on a quantum machine, together with the (natural) determination of upper bounds by simply solving the problem formulated as QUBO, also on a QPU, to the construction of an exact algorithm based on the Branch and Bound method. This will allow – against the intuition associated with the probabilistic nature of computation on QPUs – to the generation of truly optimal solutions.

References

1. Aharonov, D., Dam, W., Kempe, J., Landau, Z., Lloyd, S., Regev, O.: Adiabatic quantum computation is equivalent to standard quantum computation. SIAM Rev. **50**(4), 755–787 (2008)
2. Adamu, M.O., Adewumi, A.O.: A survey of single-machine scheduling to minimize weighted number of tardy jobs. J. Ind. Manage. Optim. **10**, 219–241 (2013)
3. Bożejko, W., Pempera, J., Uchroński, M., Wodecki, M.: Distributed quantum annealing on D-wave for the single-machine total weighted tardiness scheduling problem. In: Groen, D., de Mulatier, C., Paszynski, M., Krzhizhanovskaya, V.V., Dongarra, J.J., Sloot, P.M.A. (eds.) Computational Science - ICCS 2022. LNCS, vol. 13353, pp. 171–178. Springer, Cham (2022). https://doi.org/10.1007/978-3-031-08760-8_15
4. Bożejki, W., Grabowski, J., Wodecki, M.: Block approach-tabu search algorithm for single-machine total weighted tardiness problem. Comput. Ind. Eng. **50**, 1–14 (2006)
5. Bożejko, W., Rajba, P., Wodecki, M.: Stable scheduling of single-machine with probabilistic parameters. Bull. Pol. Acad. Sci. Tech. Sci. **65**, 219–231 (2017)
6. Potts, C.N., Van Wassenhove, L.N.: A branch and bound algorithm for the total weighted tardiness problem. Oper. Res. **33**, 177–181 (1985)
7. Potts, C.N., Van Wassenhove, L.N.: Single-machine tardiness sequencing heuristics. IIE Trans. **23**, 346–354 (1991)
8. Rajba, P., Wodecki, M.: Stability of scheduling with random processing times on one machine. Applicationes Mathematicae **39**, 169–183 (2012)
9. Rostami, S., Creemers, S., Leus, R.: Precedence theorems and dynamic programming for the single-machine weighted tardiness problem. Eur. J. Oper. Res. **272**, 43–49 (2019)
10. Uchroński, M.: Parallel algorithm with blocks for a single-machine total weighted tardiness scheduling problem. Appl. Sci. **11**(5), 2069 (2021)
11. Uchroński, M.: Test instances for a single-machine total weighted tardiness scheduling problem. https://zasobynauki.pl/zasoby/74584
12. Wodecki, W.: A branch-and-bound parallel algorithm for single-machine total weighted tardiness problem. Int. J. Adv. Manuf. Technol. **37**, 996–1004 (2008)